

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 6.19e-08 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.60e-01

Confidence level: 5.67e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,2',4,4',6,6'-Hexachlorobiphenyl</div> <div>Measured: 2.47e-08</div> <div>Predicted: 4.39e-06</div>	<div>Image not found</div> <div>1-Pentadecene</div> <div>Measured: 3.60e-08</div> <div>Predicted: 3.78e-03</div>	<div>Image not found</div> <div>3-Methoxyphenol</div> <div>Measured: 5.03e-07</div> <div>Predicted: 1.71e-02</div>
<div>Image not found</div> <div>Cyclosarin</div> <div>Measured: 6.90e-08</div> <div>Predicted: 4.71e-02</div>	<div>Image not found</div> <div>Benzene, pentamethyl-</div> <div>Measured: 9.08e-07</div> <div>Predicted: 3.16e-01</div>	